Lawrence Livermore National Laboratory

Science & Technology REVIEW

July/August 2012

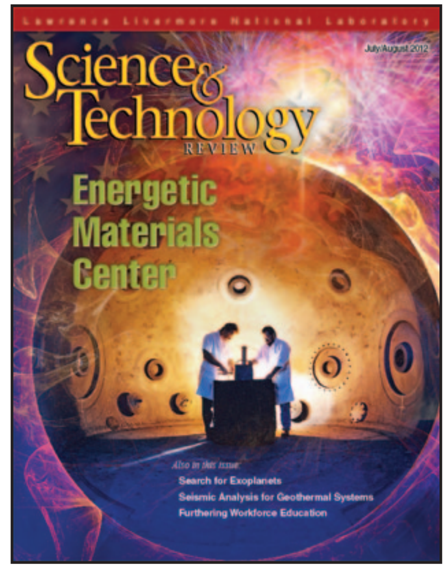
Energetic Materials Center

Also in this issue:

- Search for Exoplanets
- Seismic Analysis for Geothermal Systems
- Furthering Workforce Education

About the Cover

As the article beginning on p. 4 describes, the Energetic Materials Center (EMC) has been the focal point at the Laboratory for research and development of explosives, propellants, and pyrotechnics since its founding in 1991. The center is located at the High Explosives Applications Facility (HEAF), where the majority of high-explosives synthesis, formulation, experiment, and theory are performed at Livermore. Energetic materials are fabricated in bulk quantities at Site 300, located 24 kilometers away. The EMC staff provides expertise on energetic materials to many government and law-enforcement organizations such as the Department of Homeland Security and the Federal Bureau of Investigation. On the cover is a 10-kilogram spherical tank, one of HEAF's seven specially designed containment vessels used to safely detonate high explosives.



Cover design: Daniel S. Moore

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At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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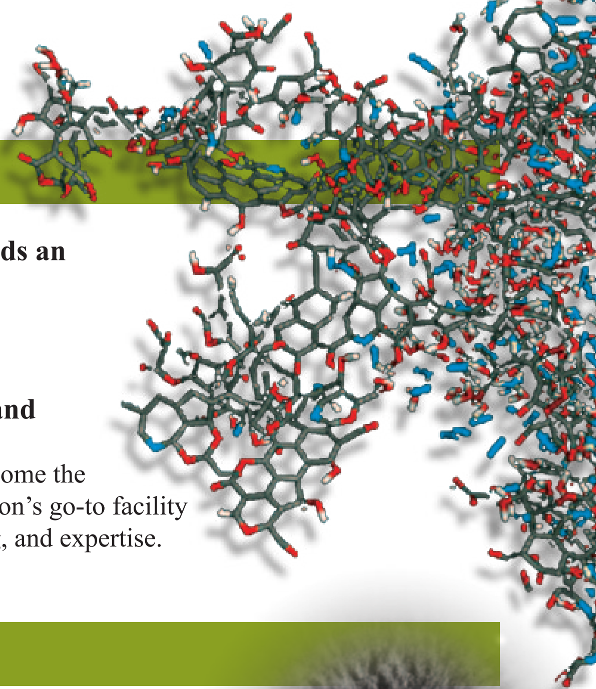
Contents



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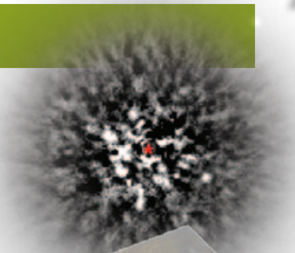
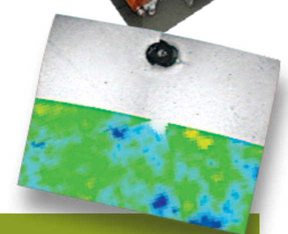
Research Highlights





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Atmospheric Warming Alters Ocean Salinity

In a paper published April 27, 2012, in *Science*, researchers from Lawrence Livermore and Australia's Commonwealth Scientific and Industrial Research Organisation (CSIRO) reported changing patterns of salinity in the global ocean during the past 50 years, marking a clear symptom of climate change. By looking at observed ocean salinity changes and the relationship between salinity, rainfall, and evaporation in climate models, the team determined the water cycle has become 4 percent stronger between 1950 and 2000—twice that projected by current-generation global climate models. With a projected temperature rise of 3°C by the end of the century, the researchers estimate a 24-percent acceleration of the water cycle is possible.

Scientists monitor salinity changes in the world's oceans to determine where rainfall has increased or decreased. "It provides us with a gauge—a method of monitoring how large-scale patterns of rainfall and evaporation (the climate variables we care most about) are changing," says Livermore postdoctoral researcher Paul Durack.

Researchers have struggled to determine coherent estimates of water cycle changes from land-based data because surface observations of rainfall and evaporation are sparse. According to the team, global oceans provide a much clearer picture. "The ocean matters to climate—it stores 97 percent of the world's water, receives 80 percent of all surface rainfall, and has absorbed 90 percent of the Earth's energy increase associated with past atmospheric warming," says Richard Matear of CSIRO's Wealth from Oceans Flagship. A change in freshwater availability in response to climate change poses a more significant risk to human societies and ecosystems than warming alone.

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Coral Reef Decline Predates Climate Change Effects

Researchers from the Scripps Institution of Oceanography at the University of California at San Diego and Lawrence Livermore reconstructed a timeline of historical change in coral reefs near Bocas del Toro in Panama and discovered that damage to the area was caused by humans as far back as the late 1800s. (Elkhorn coral photo courtesy of the National Oceanic and Atmospheric Administration.) The research appears in the June 2012 edition of *Ecology Letters*.

Using radiocarbon dating techniques at the Laboratory's Center for Accelerator Mass Spectrometry, Livermore geochemist Tom Guilderson determined the age range of degradation as reflected in species composition and fossilization and analyzed nearly a hundred coral skeletons excavated from the Bocas del Toro region. Because of the dramatic increase in bomb-produced carbon-14 concentrations in surface ocean waters that began in the late 1950s and peaked in the mid-1970s, the team was able to distinguish samples from before and after circa 1960.

The coral samples showed a decrease in the overall size of bivalves (for example, oysters, clams, and scallops), a transition from branching to nonbranching species of coral, and large declines in staghorn coral and tree oysters—once the dominant coral and bivalve on these reefs. The changes in coral and mollusk communities demonstrate that reefs near Bocas del Toro experienced substantial ecological change before 1960, and this change was likely under way by the 19th century. The team concluded that the timing of these changes implicates historical local anthropogenic disturbances such as land clearing and fishing as ultimate causes. Since the 1980s, coral cover in the Caribbean has declined by 80 percent on average and branching species have been replaced by nonbranching species. The most recent dramatic changes have been attributed to human-induced climate change.

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Graphite Enters Different States of Matter

For the first time, scientists have seen an x-ray-irradiated mineral transition to two different states of matter in about 40 femtoseconds (a femtosecond is one-quadrillionth of a second). Using the Linac Coherent Light Source, the free-electron laser at SLAC National Accelerator Laboratory, Stefan Hau-Riege of Lawrence Livermore and colleagues heated graphite to induce a transition from solid to liquid and to warm-dense plasma. Ultrafast phase transitions from solid to liquid and plasma states are important in ultrafast imaging, high-energy-density science, and the development of new material-synthesis techniques.

By using different pulse lengths and calculating difference spectra, the team was able to extract the time dependence of plasma parameters, such as electron and ion temperatures and ionization states. "We found that the heating and disintegration of the ion lattice occurs much faster than anticipated," says Hau-Riege. The research provides new insights into the behavior of matter irradiated by intense hard x rays.

Although the study ultimately serves as a breakthrough in plasma physics and ultrafast materials science, it also affects fields such as single-molecule biological imaging and x-ray optics.

(continued on p. 24)

Commentary by Bruce T. Goodwin

Energetic Materials Research Finds an Enduring Home and Mission

FEW centers of applied research have responded to the shifting needs and requirements of national security with as much agility as Livermore's Energetic Materials Center (EMC). The center's formation dates to the early 1990s, around the end of the Cold War and the collapse of the Soviet Union. This historic geopolitical shift was due in part to the significant contributions of America's nuclear weapons complex.

When EMC was founded, the way forward to sustain the nation's nuclear deterrent forces was unknown—science-based stockpile stewardship would not be launched for several years, and prospects for a significant "peace dividend" drove down defense budgets. However, a national need to preserve and advance understanding in energetic (nonnuclear, high-explosive) materials, which are fundamental components of nuclear weapons, clearly had to be sustained. As the article beginning on p. 4 describes, Lawrence Livermore leaders, in response, created EMC to manage, integrate, and advance the Laboratory's energetic materials activities.

The unusually broad support for the formation of EMC was spearheaded by three Laboratory associate directors: George Miller of Defense and Nuclear Technologies, Larry Woodruff of Military Applications, and Chris Gatrousis of Chemistry and Materials Science. Another champion of EMC was Mike Anastasio, a top deputy of Miller's, who preceded Miller as director of Livermore and later became director of Los Alamos National Laboratory.

The associate directors founded EMC with the following goals: integrate Livermore's energetic materials efforts and facilities to meet our responsibilities to the nuclear weapons enterprise and to lead the entire complex in this important technology; strengthen and build new ties to the Department of Defense (DoD), with "spin back" to the nuclear weapons complex; transition new technologies developed here to industry; and develop the next generation of energetic materials scientists through partnerships with academia. A final goal is to perform world-class science in energetic materials, including creating new formulations, testing and fabricating these materials, and developing powerful simulation software and methods. The physical home for EMC seemed obvious: the newly constructed High Explosives Applications Facility, which still houses some of the best-equipped high-explosives research and testing laboratories in the world and complements energetic materials facilities at Site 300.

EMC quickly forged new partnerships with DoD agencies, the Federal Bureau of Investigation (FBI), the Secret Service, and U.S. intelligence organizations. In 1993, the FBI tasked EMC with synthesizing the same explosives that were used by terrorists in the World Trade Center truck bombing, which killed six people and injured more than 1,000. Following 9/11, EMC began to receive important assignments from the newly established Department of Homeland Security (DHS), including conducting research activities for its Transportation Security Administration. During the two Gulf Wars, EMC also was called on by DoD agencies to enhance understanding of improvised explosive devices.

In recognition of EMC's unmatched capabilities and expertise, the National Nuclear Security Administration (NNSA) named Lawrence Livermore its High Explosives R&D Center of Excellence in 2008. Today, EMC is meeting the needs of NNSA's Stockpile Stewardship Program as well as leading a growing number of research efforts for DHS, DoD, and other federal agencies. What's more, the center also meets the needs of other major research programs at the Laboratory. For example, EMC supports the National Ignition Facility in femtosecond machining, directed energy projects, and tackling thermal-mechanical-chemical-hydrodynamic problems using Livermore's ALE3D supercomputer codes.

Meanwhile, EMC personnel help edit the international journal *Propellants, Explosives, Pyrotechnics*. They also maintain and augment the online High Explosives Reference Guide, which has hundreds of government users. The reference guide reflects the results of an important EMC activity: discovering and characterizing those everyday chemicals that could be fashioned into explosives and used in a terrorist attack.

EMC's graduate student program is flourishing. Two stellar graduates are currently professors at Texas Tech and Stanford universities. The center also leads the tri-laboratory effort for the National Explosives Engineering Sciences Security (NEXESS) Center, a program funded by the DHS Science and Technology Directorate's Explosives Division to assess threats from explosives and evaluates countermeasures. The NEXESS Center is one more example of how this Laboratory and the people of EMC are effectively responding to changing national security needs.

■ Bruce T. Goodwin is principal associate director for Weapons and Complex Integration.

A Home for Energetic Materials

Livermore's Energetic Materials Center is advancing scientific understanding of high explosives.

and Their Experts

FOR centuries, militaries have tapped the extraordinary energy locked in the molecules of energetic materials: shock waves with speeds approaching 10 kilometers per second, pressures up to 500,000 times that of Earth's atmosphere, rapidly expanding gases reaching temperatures of 4,000 kelvins, and 20 billion watts of power per square centimeter of detonation front. Since Lawrence Livermore's inception in 1952, Laboratory researchers have been among the nation's leaders in understanding, synthesizing, formulating, testing, and modeling the chemical high explosives (HE) that are an integral part of every nuclear weapon system. Such violent reactions were once extremely difficult to accurately predict, characterize, and control. However, scientific understanding of these physical and chemical phenomena has progressed significantly during the last few decades.

Since its founding in 1991, Livermore's Energetic Materials Center (EMC) has been the focal point for research and development of explosives, propellants, and pyrotechnics at the Laboratory. EMC provides oversight and direction for HE efforts at Livermore, ensuring full advantage is taken of Laboratory-wide capabilities. In 2008, the National Nuclear Security Administration (NNSA) named Livermore its HE R&D Center of Excellence because of EMC and the people and research facilities that support it. The center is located at the High Explosives Applications Facility (HEAF), where the majority of high-explosives synthesis, formulation, experiment, and theory are performed at Livermore.

Explosives, such as the well-known trinitrotoluene (TNT), react in millionths of a second, and their high-power properties are used in a variety of warheads and bombs. Propellants release similar amounts of chemical energy as explosives but over a longer period (seconds). The gases they generate are thus useful in launching objects such as artillery shells or rockets. In contrast, pyrotechnics generate only heat and light and are used to weld and cut. Pyrotechnics are more commonly found in fireworks. EMC provides expertise on all three types of energetic materials to the Department of Energy, NNSA, Department of Defense, Department of Homeland Security, Transportation Security Administration, Federal Bureau of Investigation (FBI), and other law-enforcement and government organizations.

According to EMC Director Jon Maienschein, "We needed to strengthen collaborations and integrate all the disparate high-explosives activities, bringing them together in a facility where everything—synthesis, formulation, experiment, and theory—could be done." Scientists work on theoretical models of the behavior of energetic materials; advanced simulations to better understand the fundamental physics and chemistry of energetic materials; synthesis and formulation of new energetic molecules; experimental characterization of energetic material properties and reactions; and high-speed diagnostic instruments for measuring the chemical and physical processes that occur during a detonation. (See the box on p. 7.)

Strong Growth of Simulation

The role of computer modeling and simulation in energetic materials research has grown substantially since the founding of EMC. In Livermore simulations, linear distances may vary from a fraction of a nanometer to several meters, or more than 10 orders of magnitude. Relevant timescales also range to 10 orders of magnitude, from millionths of a second to hours. Temperatures, too, can vary widely, up to thousands of kelvins. Solving multiscale problems requires massively parallel simulation tools, such as the Laboratory's supercomputers that rank as some of the most powerful in the world.

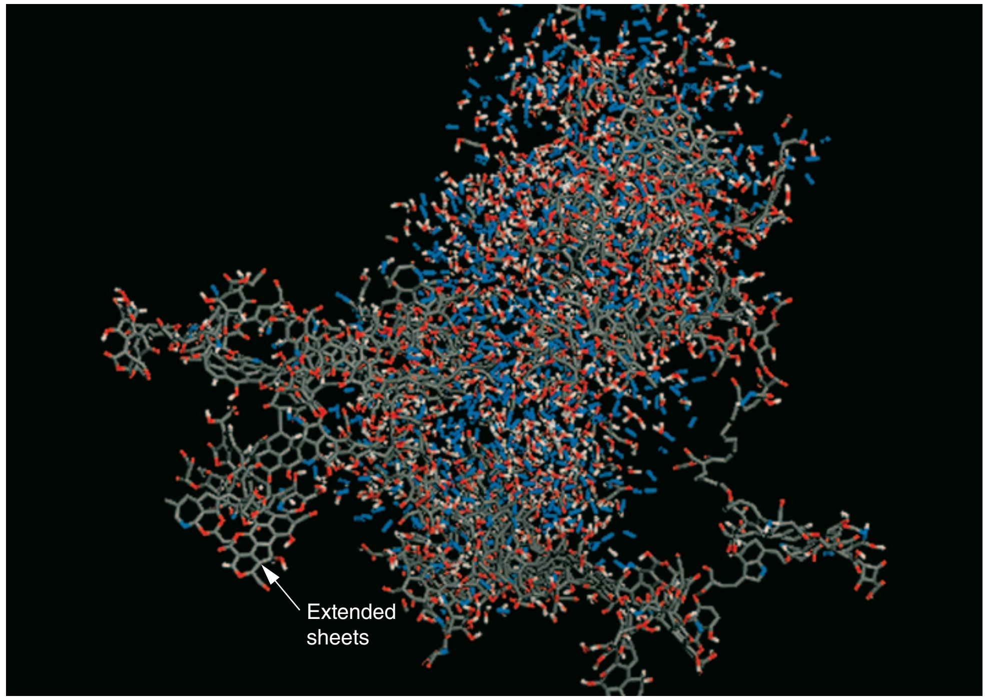
Livermore computer codes mimic the extremely rapid physical and chemical detonation processes of hundreds of energetic materials. CHEETAH is the nation's leading chemical simulation code for the performance of energetic materials, with uses ranging from nuclear weapons HE to gun propellants to improvised explosive devices (IEDs). Running on desktop computers, CHEETAH reliably runs molecular calculations based on thermodynamic properties and density parameters and converts these calculations into explosives performance measures such as detonation velocity and pressure.

The work with CHEETAH is led by computational physicist Sorin Bastea and colleagues and is based on more than a half-century of explosives experiments at Livermore. With libraries of hundreds of reactants and 6,000 products in its code, the program is used throughout the Department of Defense; version 6.0 is currently in use.

CHEETAH is linked to Livermore's hydrodynamics code ALE3D. Such a linkage, which requires hundreds of processors working in parallel, permits realistic modeling of both chemical and physical reactions across a wide envelope of detonation conditions and is invaluable in determining an explosive's safety characteristics. "ALE3D allows researchers to simulate the thermal environment of any situation," says Randy Simpson, associate program leader for Livermore's Weapons and Complex Integration Principal Directorate. "The code will track thermal expansion and chemical changes and, when an explosion finally occurs, the violence of the reaction."

Livermore codes are routinely updated to incorporate new theoretical and experimental findings. Computational physicist Larry Fried leads quantum simulations on Livermore supercomputers for NNSA's Advanced Simulation and Computing Program to strengthen the chemical and physical reaction assumptions on which CHEETAH is based. Involving thousands of microprocessors, the simulations have revealed fleeting unexpected details.

For example, simulations show that for less than 100 picoseconds, detonating high explosives act similar to a metal; that is, they become electrically conductive. Hydrogen ions become extremely mobile, while other elements remain firmly bonded to each other. In addition, simulations show that during detonation, high-explosive constituents possess characteristics of both a soup of molecules as well as a collection of high-energy ions resembling plasma. (Scientists had long debated which model was more accurate.) Finally, advanced hydrodynamics simulations using CHEETAH reveal that HE safety characteristics are highly dependent on the size of an explosive's powdered grains.



A molecular dynamics simulation shows a "soup of molecules" made by detonating the high explosive 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). The entire simulation is composed of more than 1 million snapshots in time. The results indicate that carbon (gray) is present in extended sheets, while nitrogen (blue), oxygen (red), and hydrogen (white) are mostly outside the sheets. This chemical insight is being incorporated into future versions of the CHEETAH code.

Searching for Energetic Molecules

The synthesis of new explosives with tailored properties is a cornerstone EMC activity. The work is driven by the search for molecules that yield more energy, are safer to store and handle, and are less expensive and more environmentally friendly to manufacture than current formulations. Advanced simulations make it possible to predict many material properties of new molecules, a significant improvement over the standard trial-and-error approach.

"Synthesis is both an art and a science," says chemist Phil Pagoria. For

This sequence of stop-action shots shows a bullet penetrating a sample of insensitive high explosives (IHEs) recorded at a rate of 30,000 frames per second. The bullet would have immediately detonated a more sensitive high explosives formulation on impact. The yellow cloud in the last image is unreacted IHE being expelled from the sample.

example, a chemist can attempt many multistep approaches before finding a method that produces the first few grams of a new molecule. Selecting the easiest, fastest, safest, and most environmentally friendly path requires knowledge, experience, and often the help of computer simulations. Synthesizing the first gram of an explosive may take three to six months, followed by several more months of effort to produce an optimized production process.

New molecules must pass a battery of tests that determine sensitivity to impact, friction, heat, electrostatic discharge, and shock as well as resistance to chemical decomposition. Promising molecules that pass performance and safety tests are sent to other chemists for incorporation into a mixture of ingredients, in particular binders. Additional ingredients reflect necessary trade-offs among sensitivity, performance, ease of manufacturing, safety, cost, and environmental considerations.

Synthesis and formulation chemists have helped pioneer high explosives that are remarkably insensitive to heat, shock, and impact. The most important insensitive high explosive (IHE) used in modern nuclear warheads is 1,3,5-triamino-2,4,6-trinitrobenzene (TATB), which is virtually invulnerable to significant energy release in plane crashes, fires, and explosions or to deliberate attack with small arms fire. TATB can be found in nuclear weapons, conventional munitions, and explosives used for mining and oil production. Livermore researchers developed a more

Moving beyond Nuclear Weapons

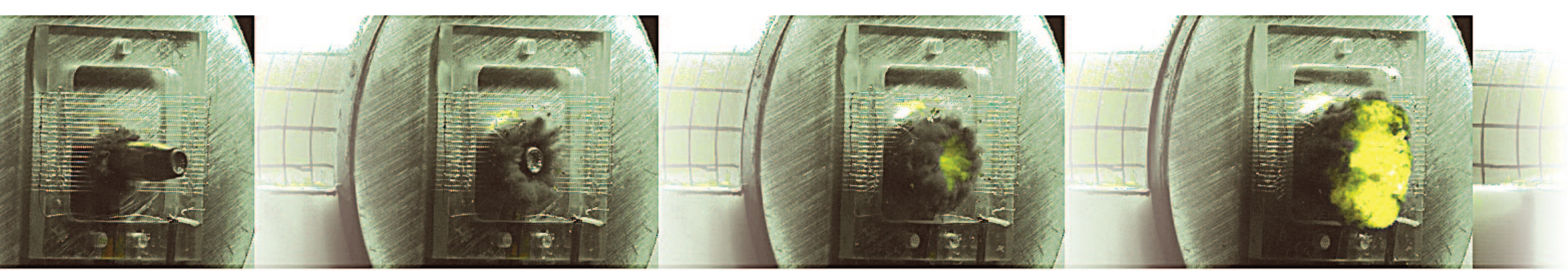
The Energetic Materials Center's (EMC's) historic emphasis has been on researching high explosives (HE) used in the main charge, booster, and detonator of a nuclear weapon's firing system. These efforts have enabled the design of and improvements to the nuclear stockpile throughout the center's history. EMC currently supports the National Nuclear Security Administration's Stockpile Stewardship Program, which ensures the safety, security, and reliability of the U.S. nuclear weapons stockpile. Toward that end, EMC researchers conduct performance and safety testing aimed at ensuring that the HE in nuclear warheads will be dependable over many decades. Routine stockpile stewardship tests examine the physical, chemical, detonation, and mechanical properties of HE taken from the nuclear stockpile.

Although HE for nuclear weapons remains a core element of scientific work, the breadth of research has grown immensely, particularly during the past decade. EMC conducts research and development for advanced conventional weapons for the Department of Defense, including new gun propellants, bombs designed to penetrate hard targets such as underground reinforced concrete bunkers, and high-speed explosive projectiles for defeating thickly armored vehicles.

As an example of new thinking for advanced conventional weapons, the Laboratory was the first to design a carbon-composite-cased munition combined with an enhanced-blast-formulation explosive. Much of the weight in today's munitions is in the steel casing. Coupled with a high explosive, the blast created by conventional steel-cased munitions can send shrapnel to distances exceeding 1 kilometer from the target, placing civilians and friendly forces at risk. Carbon-cased munitions greatly reduce collateral damage, while enabling enhanced close-in performance.

Increasingly, EMC researchers have been tasked by the Department of Defense, Department of Homeland Security, and Transportation Security Administration to investigate homemade explosives used in improvised explosive devices (IEDs) in terrorist events worldwide. This growing knowledge base includes information on detonation properties, potential safety hazards involved in their manufacture and handling, and the degree of difficulty a terrorist would face in attempting to build an IED with a particular explosive. Livermore scientists have developed an online database that includes the many explosives materials from which terrorists could build a bomb. About 1,000 federal and state scientists, engineers, and emergency responders access the database. New data are continually added as experts gain an increased understanding of terrorist capabilities and knowledge of homemade explosives.

Jon Maienschein leads the National Explosives Engineering Sciences Security Center, which applies engineering and science-based methods to assess threats and evaluate countermeasures in support of the Department of Homeland Security, Science and Technology Directorate, Explosive Division. The center is composed of scientists from Lawrence Livermore, Los Alamos, and Sandia national laboratories. One focus of the center is analyzing the vulnerability of aircraft to threats from homemade explosives. Activities include evaluating explosives formulations, including methods of initiation, detonation properties, and the probable effects on aircraft.



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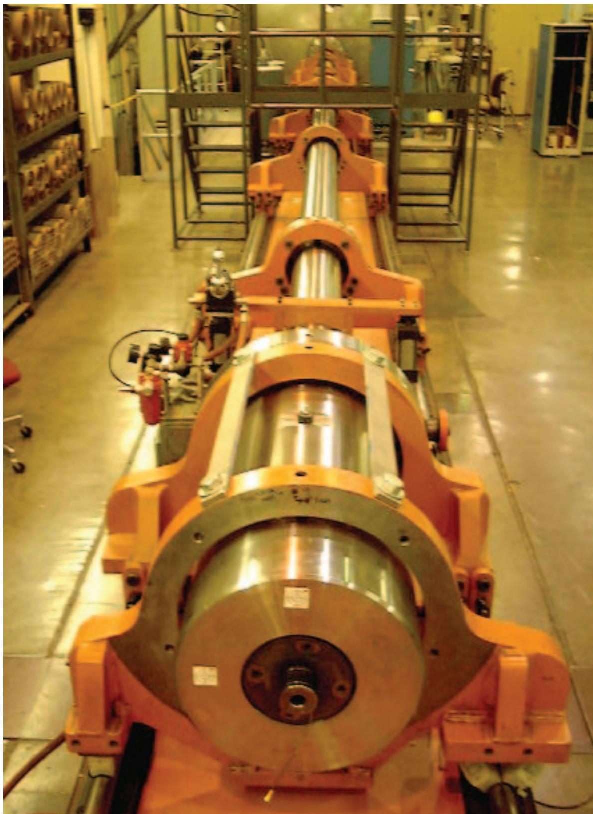

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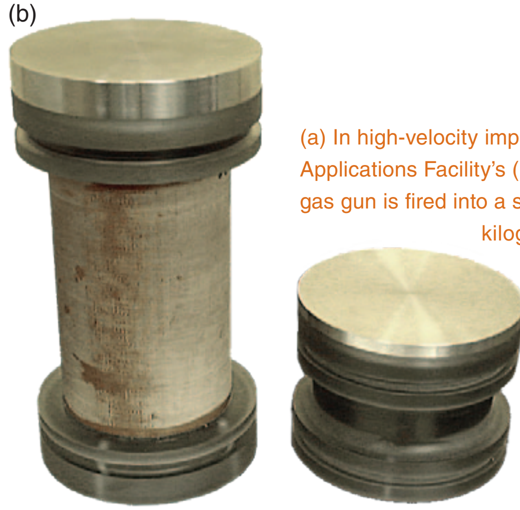

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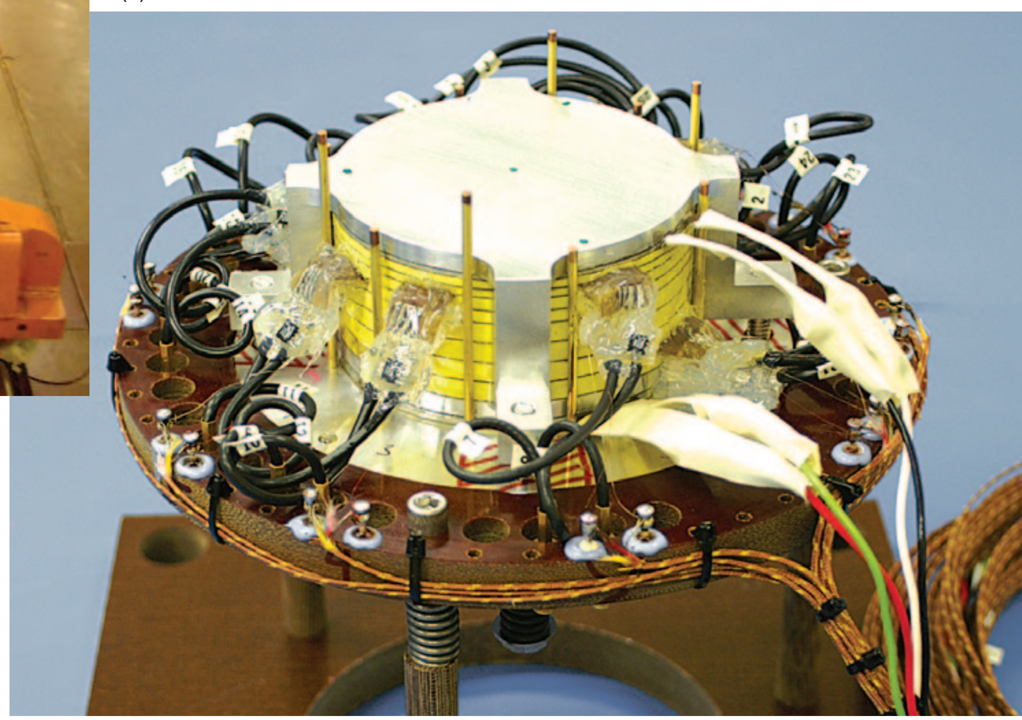


(a) In high-velocity impact studies, the High Explosives Applications Facility's (HEAF's) 100-millimeter-diameter gas gun is fired into a specially designed tank using several kilograms of propellant, with projectile velocities up to 2,500 meters per second. (b) The gun fires impactors of various sizes; smaller impactors are used for higher velocity shots. (c) The impactor hits a target composed of an outer metal layer and alternating layers of explosive (yellow) and embedded sensors.

environmentally benign and lower-cost method for producing TATB, coined the vicarious nucleophilic substitution of hydrogen method. They also developed a technique to recycle TATB crystals of superior quality from existing supplies. (See *S&TR*, June 2009, pp. 4–10.)

One IHE effort is synthesizing new molecules for use as boosters to set off the main HE charge of a nuclear device. A promising molecule is Lawrence Livermore Molecule-105 (LLM-105), which produces about 10 percent greater power than the IHE booster material ultrafine TATB. It also has greatly improved mechanical properties and performance at extreme temperatures, with safety properties similar to TATB.

For conventional munitions, LLM-172 is under development as a possible replacement material for TNT because of the latter's environmental drawbacks. LLM-172's melting point of 84°C aids processing safety because it is much lower than the temperature at which the material becomes unsafe. Livermore chemists have also developed new propellant ingredients for large guns to modify the burn rate and generate performance-improving gases. One new formulation, LLM-137, is composed of about 75 percent nitrogen, which extends the life of large gun barrels.

In addition, researchers are rethinking the very nature of new energetic materials. For example, chemist Alex Gash and materials scientist Troy Barbee are leading an effort to develop environmentally safe energetic nanolaminates that would augment or replace chemical explosives in conventional weapons. A nanolaminate is a dense solid composed of thousands of nanometer-scale layers. These materials store chemical energy in a manner similar to conventional explosives and remain inert until activated. (See *S&TR*, November/December 2008, pp. 10–16.)

Testing Explosives

Explosives tests at HEAF are conducted in one of seven indoor firing tanks. The tanks range from a 76-centimeter-diameter tank rated for 7.5 grams of TNT-equivalent explosives to a 4.9-meter-diameter tank rated for 10 kilograms. The facility also has a capability for shock compression experiments using large gas guns. For high-velocity impact studies, a 100-millimeter-diameter single-stage gas gun is fired into a specially designed tank. The gun uses several kilograms of propellant and achieves projectile velocities up to 2,500 meters per second.

A two-stage gun at HEAF fires smaller-diameter projectiles to velocities of about 8,000 meters per second. The two-stage gun is a companion to one at the Joint Actinide Shock Physics Experimental Research Facility at the Nevada National Security Site, where actinide research is conducted. Other resources include a range of guns for testing small-caliber ammunition and a microdetonics laboratory for studies at the millimeter to micrometer scale.

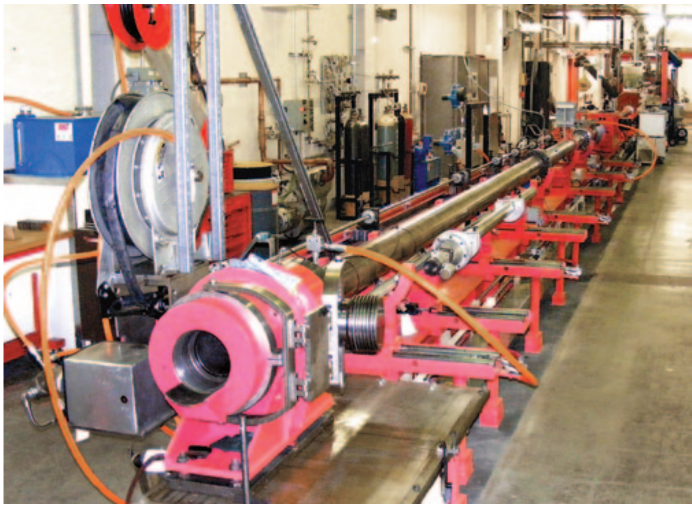
HEAF laboratories are used to characterize energetic materials for their safety, sensitivity, and mechanical and thermal stability. The detonation products of these energetic materials are determined as well. Tests are thoroughly instrumented with high-speed diagnostics including x-ray radiography, x-ray computed tomography, high-speed photography, and laser velocimetry.

"We run experiments with high-fidelity diagnostics that collect a large amount of precise data," says Maienschein. "Where we once would run dozens of experiments to obtain the information we wanted, we now need only a few, especially if we use computer simulations to design the initial experiment."

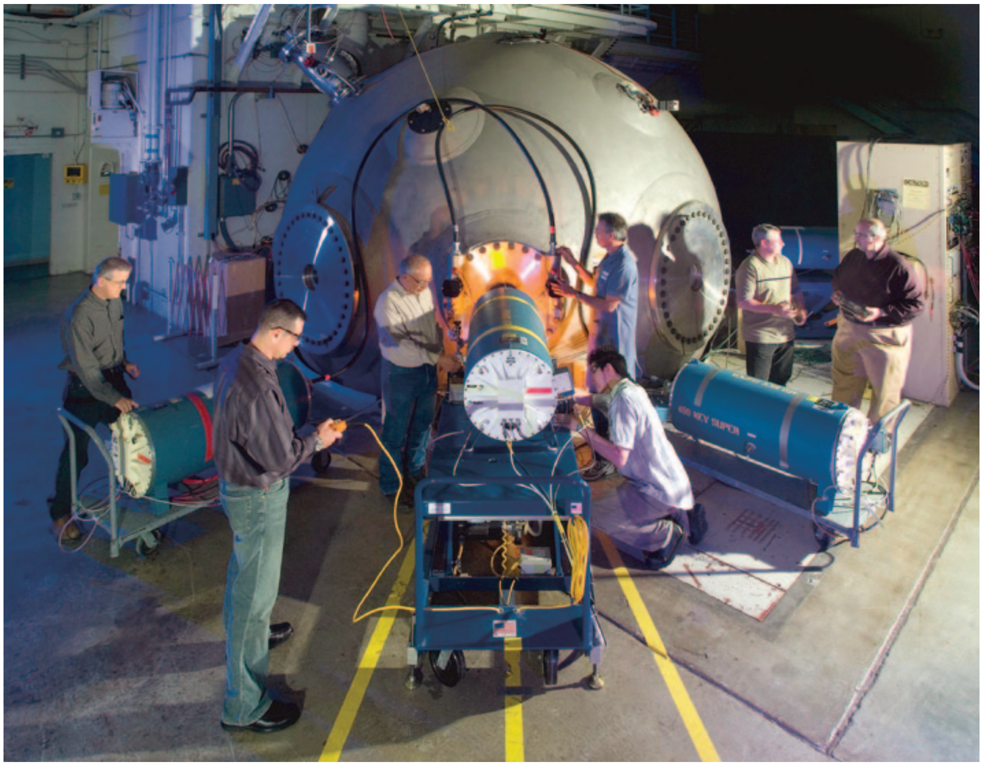
Maienschein cites long-standing efforts to develop ever-more-accurate diagnostics. One of Livermore's most important diagnostic instruments is the photonic Doppler velocimeter (PDV), which uses standard fiber optics and commercial digitizers. Easy to operate and extremely accurate, PDV records continually changing velocities by measuring the Doppler-shifted frequency of light reflected off a surface. (See *S&TR*, July/August 2004, pp. 23–25.)

Site 300 Operations

Energetic material fabrication ranges from the gram-to-kilogram scale at HEAF to hundreds of kilograms at Site 300, 24 kilometers southeast of the Labortory's main site.



In HEAF's two-stage gas gun, the first stage uses gunpowder and a piston to compress a light drive gas, typically hydrogen, to very high pressures. A rupture disk releases the drive gas into a smaller diameter launch tube, which contains the experimental projectile. The launch tube guides the projectile to the target chamber, which connects to diagnostic instruments outside the chamber.



Explosives tests at HEAF are conducted in one of seven indoor firing tanks. Here, HEAF technicians and engineers ready a test at the spherical tank rated for a maximum of 10 kilograms of trinitrotoluene- (TNT-) equivalent explosives. The blue cylinders arrayed around the tank form the Hydra x-ray diagnostic, which records a multi-image time sequence of each shot.

Fabrication activities at Site 300 include large-scale synthesis, formulation, pressing, machining, and assembly. The capability to manufacture large precision melt-cast explosives parts is unique to NNSA and the nation.

The casting of large amounts of high explosives at Site 300 is supervised by formulation chemist Sabrina DePiero and others, who work both at HEAF and at Site 300. Much of the casting work supports counterterrorism programs that test large explosive devices for determining their properties as IEDs and as part of improvised nuclear devices, which would presumably use HE along with some type of nuclear material.

Some "melt castable" explosives, such as Composition B (a mixture of TNT and RDX [1,3,5-trinitro-1,3,5-triazacyclohexane]), are gently heated and poured into molds. A team of chemists, mechanical engineers, and technicians oversees the explosives casting at Site 300's Building 827 complex, which includes a control room as well as three earth-covered cells for explosives processing. "Casting Composition B in a large kettle is similar to making caramel candy," says Site 300 Manager John E. Scott. Once melted, the explosive is poured into a mold, slow-cooled by a water bath, and later machined to the precise shape needed to accommodate instruments.

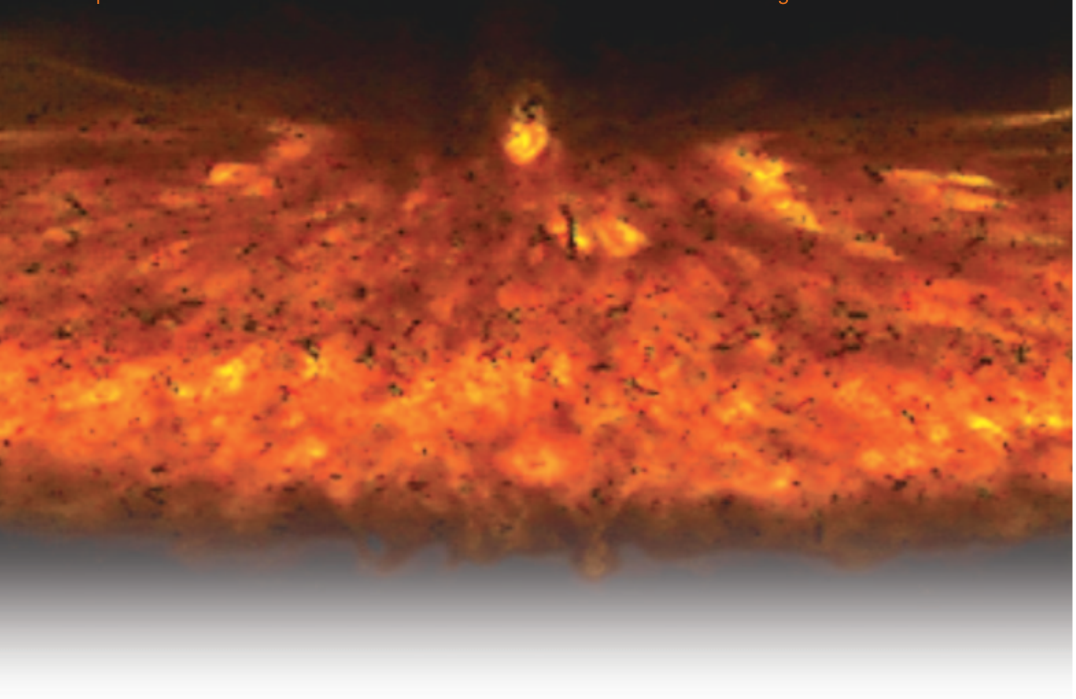
Other types of explosives are pressed into rough shapes, machined into precise shapes, and fitted with a variety of diagnostic sensors. With still other explosives, such as LX-20, binders are added to HMX (tetranitro tetraazacyclooctane), and mixing is done remotely under closed circuit cameras. The mixture can then be extruded in molds, where it cures into a solid.

Up to 45 kilograms of energetic materials are detonated at one outdoor facility, where detonation characteristics are examined for myriad applications and programs. Up to 60 kilograms of energetic materials can be detonated inside the 2,600-square-meter Contained Firing Facility (CFF), the largest indoor firing facility in the world. Energetic parts heavier than 60 kilograms are transported to the Nevada National Security Site or a Department of Defense site for testing.

CFF offers the nation's most extensive suite of diagnostic equipment for studying the detonation of explosives. Most experiments conducted at CFF support the Laboratory's stockpile stewardship efforts. The facility's flash x-ray machine, the only wide-angle penetrating radiography accelerator in the NNSA complex, captures the density and symmetry of compressed metals in 65-billionths of a second. Ultrahigh-speed rotating mirror cameras capture up to 160 consecutive frames of images at 3 million frames per second, forming a movielike record of an experiment. Testing capabilities are complementary to those at the Dual-Axis Radiographic Hydrodynamic Test Facility at Los Alamos National Laboratory, according to Jack Lowry, who leads explosives firing operations at CFF.

EMC scientists with forensic training also support the Forensic Receival Facility at Site 300. The facility is operated by

High-speed (30,000 frames per second) video captures the several-meters-wide dispersion of a thermite reaction inside HEAF's 10-kilogram spherical tank. Thermites are combinations of a metal powder and a metal oxidant. This frame occurs 1.29 milliseconds following the onset of the reaction.



The casting of large explosive charges is conducted at Site 300. For the explosive Composition B, dry chips are first placed into a melt-cast kettle and then poured into a hemispherical mold assembly and cooled. (left) Chemistry technician Aaron Fontes (shown left) and supervisor Patrick Gallagher remove the upper mold assembly, exposing the cooled, inverted hemisphere. The part's core does not contain any explosive. (below) Posing by the cooled hemispherical part are (from left) Fontes, Gallagher, formulation chemist Sabrina DePiero, engineering technicians Adriano Salamanca and George Governo, and engineer Doug Dobie. The part was then machined, joined to its twin, and transported to the Nevada National Security Site for testing.

Livermore's Forensic Science Center (FSC), where experts determine the composition and often the source of minute samples of evidence to counter terrorism, aid domestic law enforcement, and verify compliance with international treaties.

The Forensic Receival Facility is designed to ensure chain of custody of evidentiary materials if a terrorist on U.S. soil detonates an explosive. At the FBI's request, explosives involved in a terrorist event would be received, sampled, and temporarily stored at the facility. A climate- and contamination-controlled, air-filtered transportainer is dedicated to processing HE-contaminated evidence delivered to the facility following such an event. Samples would eventually be transported by a specialized van to Livermore for detailed analysis at the FSC analytical laboratories and HEAF. An FBI-led exercise in 2009 demonstrated the utility of the Forensic Receival Facility, if it should be required.

Worldwide Influence

Although much of the energetic materials research must remain classified, Livermore researchers publish 40 to 50 journal articles each year in leading international science journals. Simpson is the U.S. editor, and Livermore chemist Richard Gee is the U.S. associate editor of *Propellants, Explosives, Pyrotechnics*, which is published in Germany by Wiley-VCH. In addition, the Laboratory cosponsors the International Detonation Symposium Series, which began in 1951.

Such international exposure and academic collaboration help strengthen the expertise and influence of EMC researchers, notes Maienschein. From precise explosive devices that destroy terrorists (but not close-by civilians), to the devastating explosive power of highly penetrating bombs, to remarkably insensitive formulations in nuclear weapons, energetic materials are the focus of myriad innovative research efforts at the Laboratory.

—Arnie Heller

Key Words: ALE3D, CHEETAH, Composition B, Contained Firing Facility (CFF), Energetic Materials Center (EMC), flash x ray, Forensic Receival Facility, high explosive (HE), High Explosives Applications Facility (HEAF), improvised explosive device (IED), insensitive high explosive (IHE), National Explosives Engineering Sciences Security Center, photonic Doppler velocimeter (PDV), Site 300, Stockpile Stewardship Program, tetranitro tetraazacyclooctane (HMX), 1,3,5-triamino-2,4,6-trinitrobenzene (TATB), 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX), trinitrotoluene (TNT).

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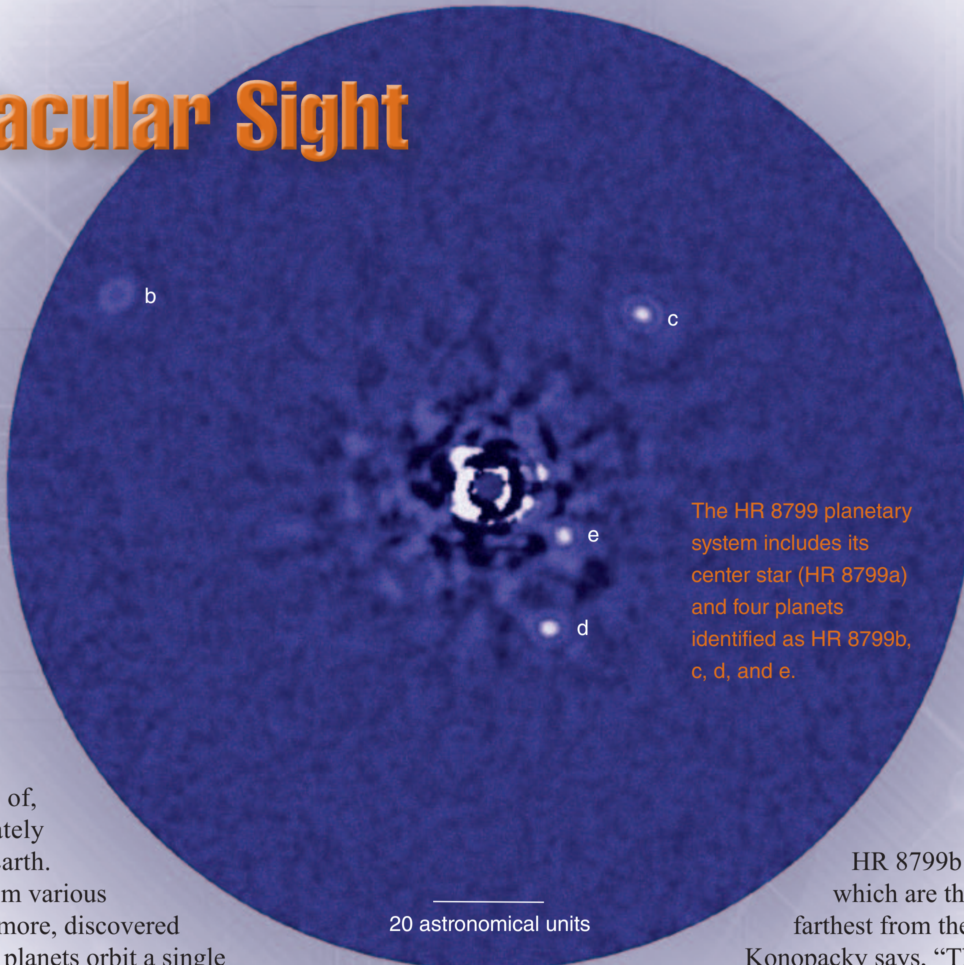
A Spectra-Tacular Sight

IN space and among the stars, astronomers and astrophysicists look for answers to the most fundamental questions regarding our existence. Earth lies in a planetary sweet spot, known as the Goldilocks Zone, where conditions are not too cold and not too hot, but just right for life to thrive. For a little more than a decade, scientists have been actively searching the vast expanse of space for solar systems with planets—called exoplanets—that are possibly similar to our own. These “sister” systems may in turn provide insight into what exoplanets are made of, how they form and evolve, and ultimately whether life exists in places besides Earth.



The HR 8799 planetary system includes its center star (HR 8799a) and four planets identified as HR 8799b, c, d, and e.

In a landmark study, researchers from various institutions, including Lawrence Livermore, discovered a distant solar system in which several planets orbit a single star known as HR 8799, a formation similar to Earth’s solar system. Livermore astrophysicist Bruce Macintosh says, “We looked at approximately 400 stars during our search for exoplanets, and what we found here is extremely rare.” Interestingly, the four planets within the system are three to seven times the mass of Jupiter and orbit at a distance of 15 to 70 astronomical units (AU) from HR 8799—where 1 AU is the distance from Earth to the Sun, or nearly 150 million kilometers. “It’s a mystery how planets that big form so far away from their parent star,” says Macintosh. These giant planets orbiting on the outside of the system could indicate that smaller, Earth-like planets exist closer to the star.

This year, Macintosh and former Livermore postdoctoral researcher Quinn Konopacky worked in collaboration with scientists from the National Research Council Canada’s Herzberg Institute of Astrophysics and Lowell Observatory in Arizona to characterize the planets in the HR 8799 system. Using the OSIRIS integral field spectrograph and a high-powered telescope at Keck Observatory on the island of Hawaii, Macintosh and colleagues measured the spectra emitted to determine the plantets’ atmospheric makeup. In particular, they analyzed planets HR 8799b and c, which are the two farthest from the star. Konopacky says, “This research represents the first time that molecular features have been seen at such a detailed level within exoplanets.” The team’s work was funded by Livermore’s Laboratory Directed Research and Development Program.

Without a Doubt

Direct spectroscopy of exoplanets is extremely challenging for several reasons. “Because light from the star is so much brighter than light from the planets, we have to find ways to remove the starlight to extract the planet signal,” says Konopacky, now a postdoctoral fellow at the University of Toronto. The problem is further compounded by Earth’s atmosphere, which scatters light, making objects even harder to differentiate.

OSIRIS and the 10-meter Keck telescope proved to be ideal tools for overcoming these barriers. OSIRIS works in conjunction with the telescope’s precise adaptive optics system to sample a rectangular area of the sky, separately recording the individual spectra of objects within its field of view at high resolution. One benefit of OSIRIS is that researchers can take such spectrographic measurements without having to line up the instrument directly with the object they are analyzing. The team also developed advanced image-processing algorithms and filtering techniques to more accurately distinguish the planet from the scattered starlight.

Different molecules absorb light at different wavelengths; thus, the light emitted from a planet directly correlates to the molecules in its atmosphere. "Molecular features have a specific spectral fingerprint that indicates the presence of a molecule without ambiguity," says Macintosh. However, scattered starlight mimics the signals of interest and manifests itself as "speckles" in the images, effectively masking the planetary spectra.

To solve this problem, Macintosh developed an algorithm to help suppress and remove the scattered starlight. Spectrographic data are represented in "cubes," where the *x* and *y* axes show the image of the field, and the *z* axis consists of slices of light at different wavelengths. Over time, the star's and planet's positions remain fixed within the cube, while the speckles appear farther from the center of the star at longer wavelengths. (See the figure below.) "We take advantage of how the positions of the speckles change with wavelength to more easily remove them from the data," says Macintosh. The code accounts for the speckles' brightness and changing position through the cube. It then subtracts them out, while maintaining the integrity of the planet's signal. Macintosh adds, "The problem with previous algorithms is that they remove 90 percent or more of the speckle light, and with it, 20 percent of the light from the planet in a biased way." This new linear algorithm is powerful because of its simplicity. It removes about 50 percent of the noise but does not inject any bias into the measurement of the planet.

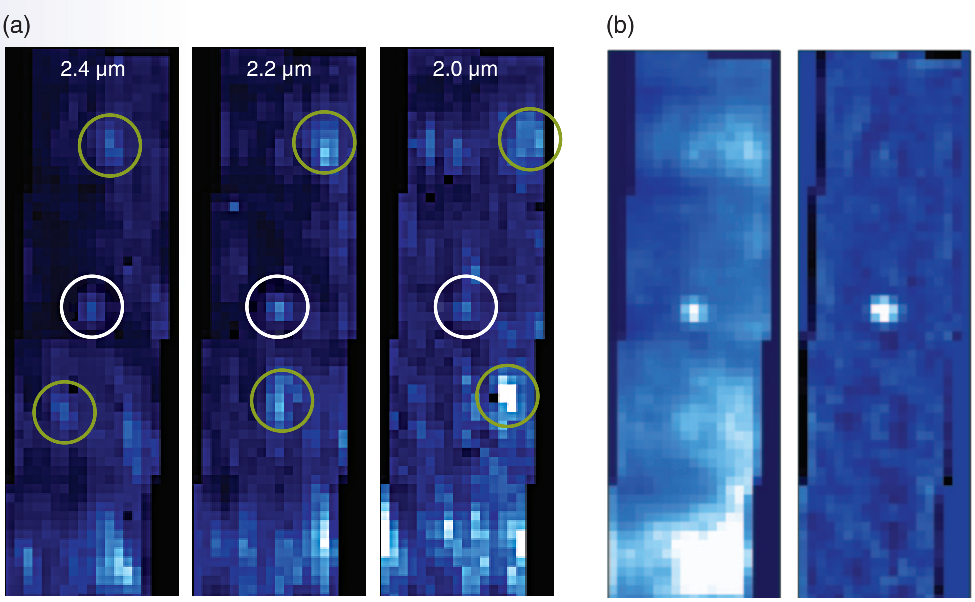
Data were collected over 2010 and 2011 at the full spectral resolution provided by OSIRIS and input into computational models for analysis. Armed with the new filtering techniques, the team reduced and analyzed all the spectra and discovered the HR 8799 planets have high concentrations of water and carbon monoxide, uncharacteristic of giant gas planets in our solar system.

Surprise, Surprise

One theory for how planets form, including giant gas planets such as Jupiter and possibly those in the HR 8799 system, is through core accretion. In this process, a cloud of interstellar gas, comprising mostly hydrogen, forms into a star and a protoplanetary disk. Cooler regions on the outskirts of the disk contain icy planetesimals, made from molecules including frozen water and carbon monoxide, which stick together to create a planet's core. When the core's mass is big enough, it sucks excess gas from the cloud around it to form a giant gas planet that contains more of the materials in the form of solid ices (including oxygen, carbon, and nitrogen). In contrast, planets such as Earth are too small, and formed too late, to pull in gases from the surrounding cloud and thus have a wholly different chemical composition.

As a result of this formation process, giant gas planets primarily comprise hydrogen with a smattering of heavier elements such as carbon. As the planets cool, most of the carbon forms into methane. Surprisingly, the planets in the HR 8799 planetary system have more carbon monoxide than methane. Other, more refractory elements form dust clouds. Of interest is that the HR 8799 planets have much thicker dust clouds than predicted by older models.

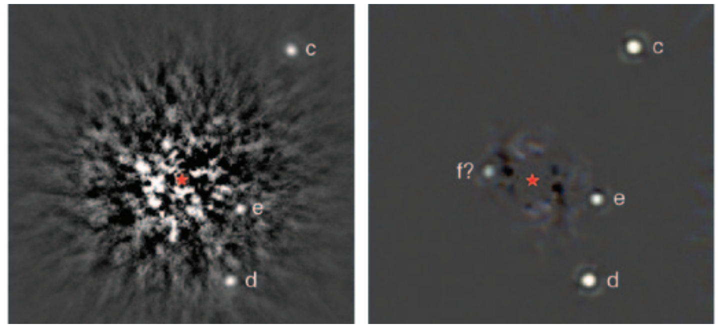
"Results like this tell us that something unusual is happening," says Macintosh. "Conditions within the planets are causing their atmospheres to circulate, pushing the methane down and the carbon monoxide and clouds up." The large amounts of carbon



(a) Three wavelength "slices" of data are taken from the OSIRIS integral field spectrograph at near-infrared wavelengths ranging between 2.0 and 2.4 micrometers (μm). The *x* and *y* axes represent position, and the star is to the right (not pictured). The speckle artifacts (yellow circles) are further from the star at longer wavelengths, while the planet (white circle) stays fixed, thereby allowing researchers to remove the speckle noise and enhance the planet. (b) These two images show a combination of about 200 wavelength slices between 2.0 and 2.4 μm before (left) and after (right) the speckle artifacts are removed. (Courtesy of Quinn Konopacky, University of Toronto.)

monoxide suggest that more carbon and oxygen were available when the planets formed. Macintosh says, "Excess oxygen and carbon in the HR 8799 planets means they probably formed through core accretion, which is a process that can theoretically also make Earths."

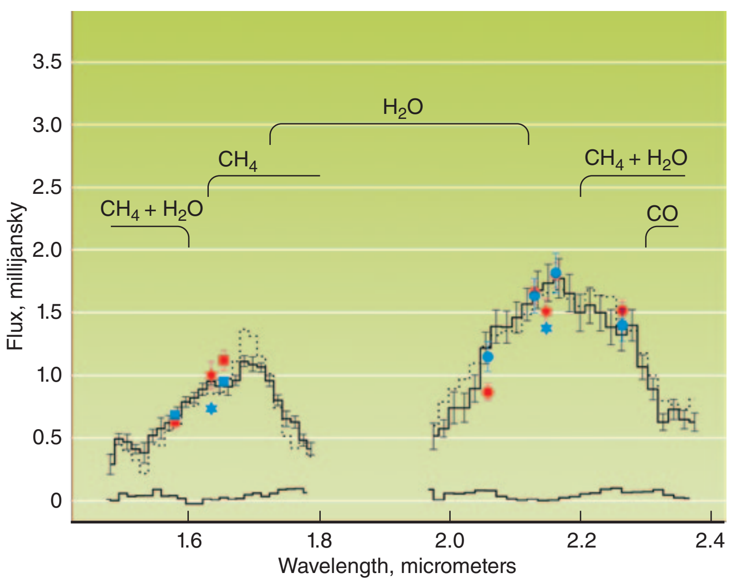
Konopacky is continuing to study the atmospheric phenomena in more detail. "We're using spectrographic measurements to determine the metallicities and ratio of carbon to oxygen within the planets," he says. Recent analysis of the data indicates that planet HR 8799c is hotter than HR 8799b and contains even more carbon monoxide. "We're still in the process of determining exactly what the molecular features are telling us about the planets and the potential implications of those findings," says Konopacky. "We may be heading into really exciting territory."



Side-by-side images of HR 8799 compare the image contrast achieved with the Keck telescope (left) to simulated results from the Gemini Planet Imager (GPI) in Chile (right). With GPI, a hypothetical exoplanet labeled "f" is clearly visible. (Courtesy of Christian Marois, National Research Council Canada.)

Are We Alone?

The holy grail of exoplanet research would be to find a small, rocky planet with a similar chemical composition to Earth orbiting a star. However, Earth-size planets are 10,000 times fainter than their giant planet counterparts and much too small to view with current technology. More advanced, precision instruments will be required to observe these planets at high enough resolutions that they can be studied in detail.



This plot shows the near-infrared spectrum of planet HR 8799b as captured by the OSIRIS spectrograph and Keck telescope in Hawaii. HR 8799 planets have high concentrations of water (H_2O) and carbon monoxide (CO). (CH_4 is methane.) The solid line with error bars shows the measured spectrum, while the dotted line indicates the spectrum before the speckle noise is removed. The solid lines at the bottom depict errors in measurements of simulated test planets with known spectra, which enable researchers to check for biases in the analyzed data. Colored symbols show measurements made with the Keck telescope's NIRC2 camera. (Courtesy of Travis Barman, Lowell Observatory.)

Toward this end, Macintosh is spearheading an international effort to install the Gemini Planet Imager (GPI, pronounced gee-pie) at the Gemini South telescope in Chile. (See *S&TR,* March/April 2008, pp. 4–10.) The sensitivity of GPI is much higher than any other instrument for directly observing distant objects. With GPI's sophisticated and improved adaptive optics system, astronomers will be able to detect objects more than 10 million times fainter than their parent stars. The system also includes a spectrograph for measuring atmospheric data. The spectrograph is an improved version of OSIRIS, and a team at the University of California at Los Angeles is tuning it specifically for hunting planets. "GPI will allow us to make many hundreds of observations for building our understanding of how planets form and evolve," says Macintosh. Looking up through Earth's atmosphere on an 8-meter telescope, GPI will still not be sensitive enough to see an Earth-like planet, but it should enable researchers to discover dozens of previously hidden giant planets.

With improved planet-detecting capabilities, will sleuthing astronomers find that Earth is one among many of its kind or the exception to every rule? Only time will tell whether the search for other Earths will lead to the discovery of life on other planets.

—Caryn Meissner

Key Words: core accretion, exoplanet, giant gas planet, HR 8799, Keck telescope, OSIRIS integral field spectrograph.

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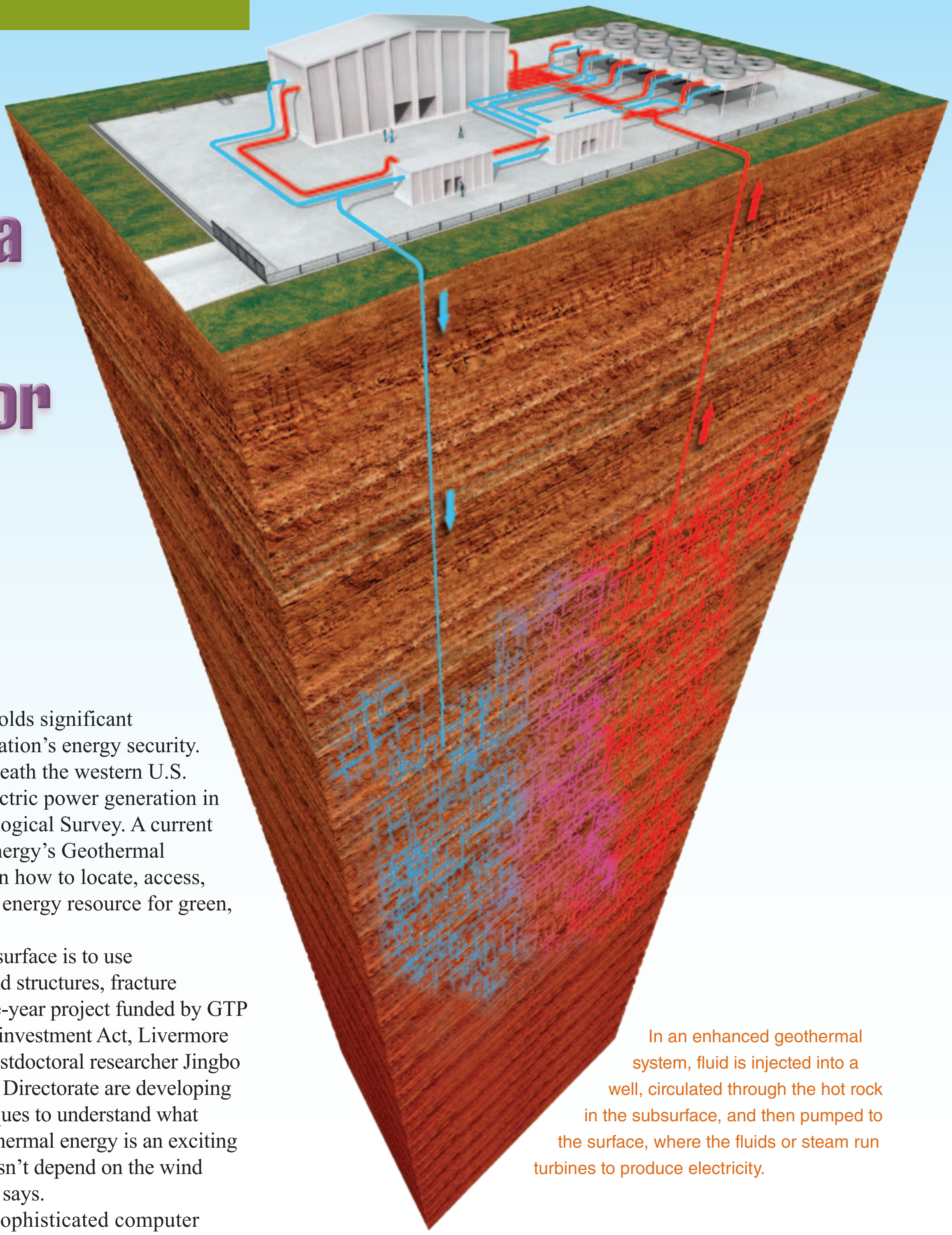


Seismic Data Pinpoint Fractures for Geothermal Energy

THE hot rock in Earth's subsurface holds significant potential for helping to ensure the nation's energy security. In particular, geothermal resources beneath the western U.S. could provide a large portion of the electric power generation in the country, according to the U.S. Geological Survey. A current research focus of the Department of Energy's Geothermal Technologies Program (GTP) is to learn how to locate, access, and effectively use this vast renewable energy resource for green, baseload, electric generation.

One method of interrogating the subsurface is to use microseismic events to map underground structures, fracture networks, and fluid pathways. In a three-year project funded by GTP through the American Recovery and Reinvestment Act, Livermore seismologist Dennise Templeton and postdoctoral researcher Jingbo Wang of the Physical and Life Sciences Directorate are developing advanced microseismic analysis techniques to understand what happens beneath Earth's surface. "Geothermal energy is an exciting renewable energy source because it doesn't depend on the wind blowing or the sun shining," Templeton says.

Templeton's team is developing a sophisticated computer algorithm to better extract information from seismic data and ultimately promote the development of cost-effective enhanced geothermal systems (EGSs) that can draw energy from the subsurface and convert it for electric generation. Jeff Roberts, who leads the Laboratory's Renewable Energy Program, says, "Our hope is that we can expand our use of seismic information to understand fluid injection and where that fluid travels in the subsurface."

In an enhanced geothermal system, fluid is injected into a well, circulated through the hot rock in the subsurface, and then pumped to the surface, where the fluids or steam run turbines to produce electricity.

Traditionally, power plants produce geothermal energy only in high-temperature locations where naturally occurring interconnected cracks are filled with hot water or steam. However, much more geothermal energy is located in dry or impermeable rock, where water or a network of cracks may not be present. The temperature of Earth at a depth of 3 to 10 kilometers is highly variable but can exceed 300°C. EGS technology can be used to enhance existing fractures or create new ones and introduce water into these hot subsurfaces, thereby expanding the number of viable geothermal sites. Once an underground reservoir of water-filled cracks is created, power plants at the surface can either directly produce steam or use the geothermally heated water to create steam, which then turns the turbines that power generators.

Matched Field Processing

Creating and maintaining an underground reservoir, however, can result in the occurrence of microseismic events. Livermore researchers are providing better insight to the development and evolution of an EGS reservoir with the adaptation of a signal-processing technique called matched field processing (MFP). MFP was originally developed by the underwater acoustics community for detecting and tracking sources of underwater sound.

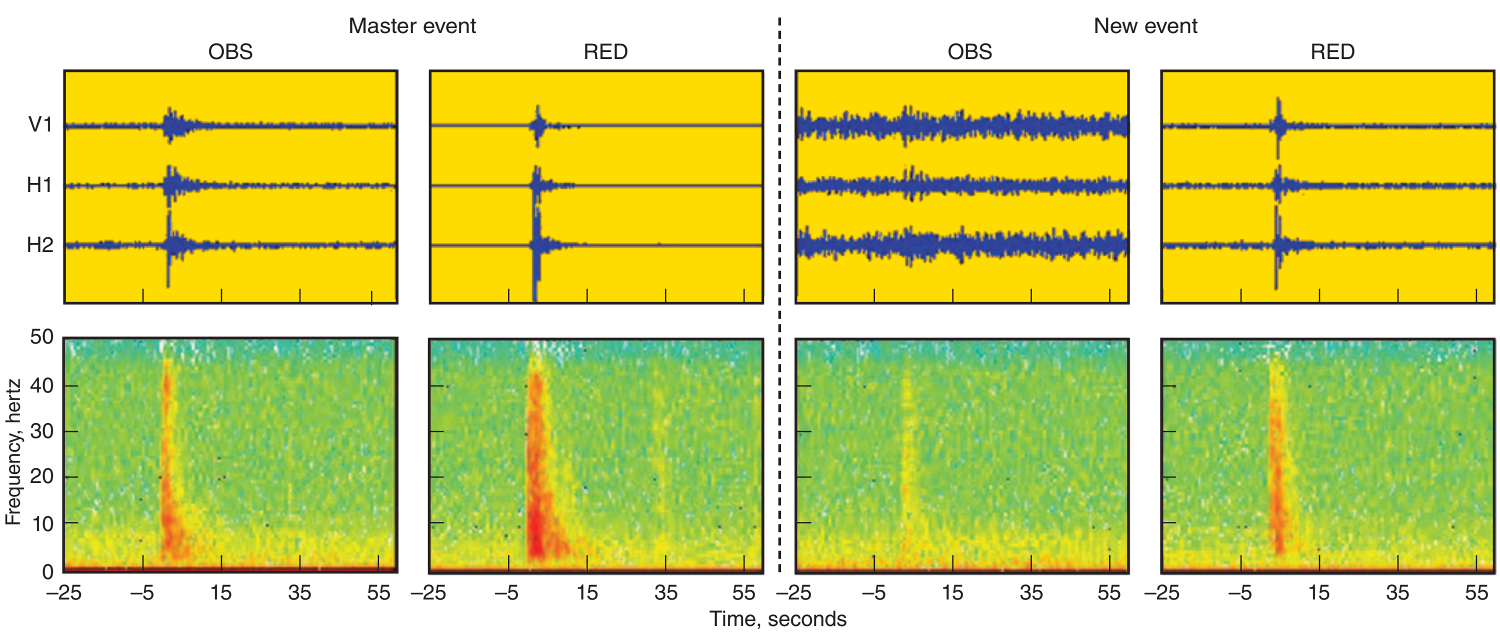
Dave Harris, former program manager for nuclear explosion monitoring and another member of Templeton's team, was among the first to adapt MFP for use with seismic data in an effort to distinguish legitimate mining explosions—multiple charges set up in a series known as ripple fire—from possible nuclear explosions. Harris says, "In geothermal research, we can use MFP to detect and map the distribution of microearthquakes produced by fracture growth. In this way, we can determine where injected water has traveled and how far a fracture has extended." These microearthquakes have tiny seismic signals, many of which have overlapping waveforms when recorded on a seismometer. Templeton emphasizes that the team is measuring very small events that people usually do not feel.

Master Events Serve as Templates

The most successful use of the MFP technique is empirical—that is, observed signals from previously detected microearthquakes serve as templates to look for new events. "Essentially, we break a subsurface area into a collection of cells, and a surface network of seismometers is used to produce a waveform pattern," says Harris. "We then compare the observed data against the waveform pattern for each cell. This comparison through all cells enables us to build a seismicity map of the rock volume surrounding an injection well."

Between November 2009 and December 2010, Livermore seismologists applied empirical MFP to continuously recorded data obtained from seismic stations in the Salton Sea Geothermal Field in Imperial County, California. The regional earthquake catalog listed 1,536 known seismic events in the study area. "We looked through all the events and found 231 events to use as master events," says Wang.

Templeton processed both the master events and the incoming seismic data (at discrete time intervals) and then matched the amplitude and phase of the incoming seismic data with the



In this comparison of seismic signals of a master event and a newly detected event recorded at the Salton Sea Geothermal Field in California, the top plots show three-component (one vertical, two horizontal) seismic records of ground motion as a function of time at two seismic instruments: OBS and RED. The bottom plots show the frequency content of the vertical component of ground motion as it changes with time. Note how the seismic signal of the new event at station OBS is extremely small compared to the background noise.

Livermore seismologist Dennise Templeton (left) and postdoctoral researcher Jingbo Wang install seismometers at AltaRock Energy's Davenport Newberry Enhanced Geothermal System Demonstration Site near Bend, Oregon. (Photo courtesy Pete Erickson/*The Bulletin*.)

precomputed master templates. "We identified 5,357 events in our study area that had magnitudes between 0.0 and 1.1 on the Richter scale, most of which had been previously unrecorded," Templeton says. The Richter scale (used to quantify the energy contained in an earthquake) is logarithmic—a logarithm is a number that shows how many times a base number (such as 10) must be multiplied by itself to produce a third number (such as 100)—so the scale does not start at zero. A –2 event, for example, is the equivalent of the shock generated by dropping a gallon of milk or a brick on the floor. The MFP technique has proven useful in identifying many more seismic events than are recorded in traditional earthquake catalogs. Detecting such low-magnitude events is important for obtaining an early indication of where injected fluids are traveling and determining the fracture network.

A more ambitious approach being investigated is to calculate waveform patterns using a sophisticated geologic model of the subsurface and high-performance computing resources. These synthetic master events would show how a modeled earthquake might look at a specific location on Earth's surface. The modeled earthquakes would then be used to create synthetic master templates.

In an effort to apply MFP to an existing EGS site, Livermore researchers have formed a working partnership with AltaRock Energy, Inc., a renewable energy production and technology company that uses innovative technologies to turn the natural heat within Earth into electricity. The Livermore team has installed Laboratory-owned seismometers at AltaRock's Davenport Newberry EGS Demonstration Site near Bend, Oregon. The Newberry project seeks to demonstrate the viability of improved technology to create geothermal reservoirs that can extract heat from the subsurface in locations where high temperatures can be reached by conventional drilling.

Wang is responsible for processing the preliminary MFP data and analyzing the results to better image the fracture network using the large number of newly identified events. "When we screen MFP detections, we filter out false detections in a predefined frequency band," she says. "We are interested in smaller events because we believe they point to small fault slips and will provide us with a detailed image of the fracture network."

The physical fracture process is complicated and not well understood. With geothermal energy extraction, injected water causes both physical and chemical changes. For example, as water is injected into the reservoir, the subsurface pore pressure increases, which can decrease the static frictional resistance on nearby faults, thereby facilitating seismic slip in the presence of an existing deviatoric stress field. Wang says, "We need a complete picture of the fracture network to help us understand this complex process so we can develop a more realistic model for optimal reservoir design."

Instead of drilling a monitoring well to identify microseismic events in a geothermal reservoir, the researchers use MFP to analyze the data provided from surface seismometers to image the fracture network. "Industry will benefit from this alternative, low-cost, microseismicity mapping method," Wang says.

Templeton notes, "At this early stage, the simulations are written in a Java program and run on my desktop. However, the opportunity exists to develop software for operators of EGS sites to use in identifying fractures and adjusting a well's water pressure without the need for special training in signal-processing algorithms or seismology."

The Livermore team's research is aimed at making geothermal resources a viable energy solution. "We could provide significant baseload electric generation for the entire country for hundreds of years, if we extract a small fraction of the geothermal energy at depth," says Roberts. "It's a phenomenal low-carbon renewable resource."

—*Kris Fury*

Key Words: earthquake, enhanced geothermal system (EGS), matched field processing, microquake, renewable energy, seismicity.

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“The foundation of every state is the education of its youth.”

—Diogenes Laërtius

Employees Keep Up with the Times

THE times keep changing, requiring employees to keep up with their own rapidly evolving fields—whether it’s mechanical engineering, computer science, biomedical informatics, or organizational management. At Lawrence Livermore, the Education Assistance Program helps promote a workforce that has the necessary skills and knowledge to address mission-critical activities. Kathy Zobel, program leader for the Education Assistance Program, says, “The Laboratory has always had to compete with private employers for workers with advanced skills, but even more significant is the need for constant skills growth and development. In particular, in scientific and engineering communities, where the bar can be raised overnight, ongoing opportunities to learn are a necessary strategy for survival.”

Livermore’s senior management agrees. Dona Crawford, associate director for Computation, says, “Employee development is advantageous to all areas of the Lab, but it is of paramount importance in computing, where the technologies are constantly evolving. Our vitality depends on a vibrant, skilled, productive, dynamic workforce.”

Forging Links with Universities

Since the early days of its existence, the Laboratory has supported further education for its employees. In the 1960s, Laboratory cofounder Edward Teller worked with the University of California (UC) at Davis to create the Department of Applied Science. That connection, along with another forged later with Stanford University, has endured and strengthened. In the 1970s, Livermore, UC Davis, and Stanford created a microwave link to offer graduate classes on site to Livermore engineers and computer scientists.

Over the past decade, 355 employees have participated in B.S., M.S., M.B.A., and Ph.D. programs, 61 in A.A. and A.S. programs, and 180 in certificate programs. Nearly 210 employees have obtained degrees, with many others now in progress. Employees also have opportunities to enroll in occasional work-related classes to enhance their skills without entering degree or certificate programs.

Zobel notes that advanced degrees, in particular, lead employees to provide ever-more sophisticated technical contributions—a requirement for a premier research and development organization such as Livermore. Since 2003, 70 percent of those receiving advanced degrees through the Education Assistance Program have been promoted or had other major career advancements. Monya Lane, associate director for Engineering, notes, "When these employees become involved in further education, they not only improve their own skills but also raise the technical level of the Engineering Directorate overall." She adds that some individuals who have continued their education at the Laboratory began their careers as engineering technicians and eventually became senior managers.

For example, Donald Boyd, principal associate director for Operations and Business, joined Engineering in 1977 with an M.S. in engineering from Massachusetts Institute of Technology. He went on to obtain a Ph.D. in materials science from UC Davis, using resources provided by the continuing education program. This commitment helped him rise through the ranks within Engineering and later at the Pacific Northwest National Laboratory. From his current position as a senior Livermore manager, Boyd encourages interested staff to simultaneously continue their education and their careers. "The Education Assistance Program is a great resource for career development that I heartily support," he says.

The Laboratory also provides tuition assistance for qualified employees. To apply, employees turn in education plans to the Student Policy Committee for review and approval. Course work and degrees can be obtained from regionally accredited institutions, from UC Berkeley to the University of Alabama. Degrees can be completed concurrently with full-time employment at the Laboratory. Employees may also request tuition assistance to take two job-related classes a year in a wide range of fields.

But it's best to let those who have "been there, done that" speak to the experience.

Get a Job, a Ph.D., or Both?

When Tim Dunn interviewed at Livermore in 1998, he had just received his master's in aeronautical and astronautical engineering from the University of Illinois. He was undecided whether to get a job or continue his education, but as it turned out, he didn't have to choose. Through the Education Assistance Program, he earned a Ph.D. in mechanical and aeronautical engineering from UC Davis, graduating in 2011.

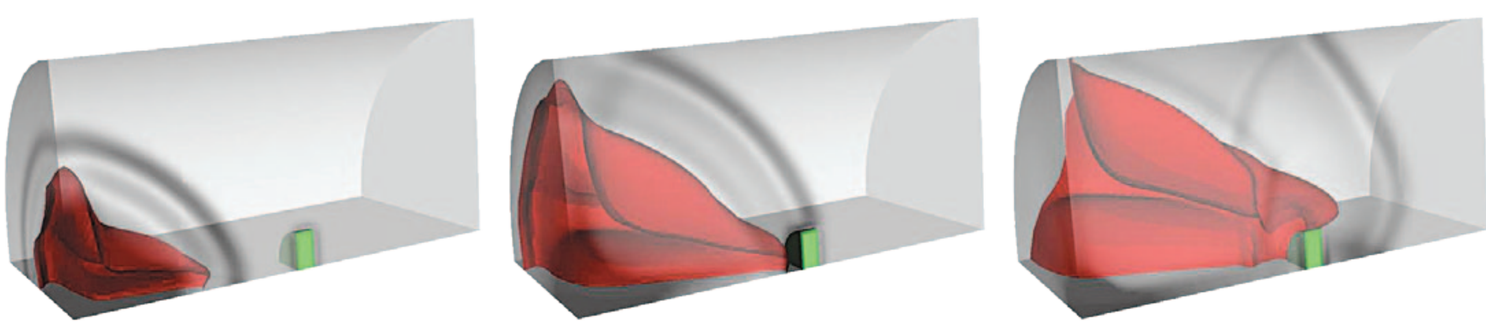
Earning a doctorate degree is a challenging process, and even more so when the student works full-time. However, in Dunn's case, the process was made easier with the Laboratory's assistance. Dunn explains, "Before I enrolled in the Ph.D. program, I took a couple of Davis classes to see if learning through the TV link would work for me. Those classes, combined with the ones I'd completed for my master's, transferred over, which shortened the process."

In his Ph.D. work, Dunn turned to a project he already supported: the ALE3D code. ALE3D is a two- and three-dimensional multiphysics numerical simulation tool for examining hydrodynamics and structures. Scientists use ALE3D to model detonation, deflagration, and convective burn processes of high explosives, propellants, and more. The code includes a multiphase portion for modeling mixtures of solids, liquids, and gases. For his dissertation, Dunn created new algorithms to model multiphase flows, extending ALE3D's capabilities. He says, "Modeling explosives is one application of this research that is of interest to the Lab. An explosive consists of a granular solid, infiltrated with gas. An explosive reaction can result in complex interactions between the gas and solid phases. Researchers want to understand this phenomenon in more detail."

While obtaining a Ph.D., Dunn depended on the Laboratory's Education Office for assistance. "I would bring the staff my completed course work assignments, and they would time stamp and fax in my work," he says. "The staff also proctored my exams and helped with paperwork. It was a great program from which I benefited."

Exploring New Fields

Biomedical engineer Haiyin Chen came to Livermore from Johns Hopkins University as a postdoctoral researcher in 2009. What drew her to Livermore, and what helps keep her here, is the

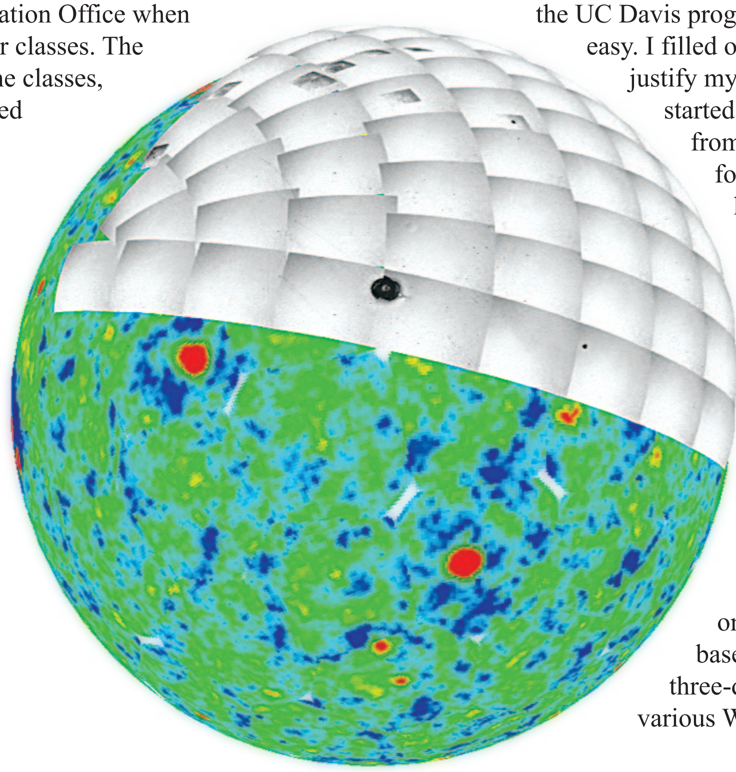


Tim Dunn created a multiphase flow capability for the hydrodynamics code ALE3D. In the simulation shown here, a high-pressure gas mixed with inert particles sends a shock into a steel plate (green). The dark shadows indicate the shock front, and the red contour is the particle front.

range of research conducted and the opportunities to participate. "The Lab is a wonderful place to work—one can continue to grow and add to one's original skill set," says Chen. "The Education Assistance Program is an important benefit offered by the Lab to its employees. I can apply new skills learned in the classroom to my present job, enhancing my contribution."

Before coming to the Laboratory, Chen's research focused on neural control of movements, a field that blends neuroscience, control theory, and computation. Thanks to the Education Assistance Program, she has added bioinformatics to the knowledge base she brings to her projects. She explains, "One of my first projects at the Lab involved examining the accumulation of starch in algae cells in a microfluidics device. Working on that project, I realized a revolution was happening in genome science as a result of breakthroughs in high-throughput sequencing technologies. I already had a keen interest in bioinformatics, particularly in mining genomic sequencing data, and I wanted to learn more and apply bioinformatics to my work in biology."

With her group leader's encouragement, she researched educational programs and discovered that Stanford offered a graduate certificate in biomedical informatics. The short course of study focuses on understanding techniques for analyzing biological data from recent genomic research. This past June, Chen completed the course requirements, working at her own pace and viewing the Web-based lectures on evenings and weekends. "My upper management was very supportive, as was Kathy," says Chen. "I contacted the Education Office when I needed to sign up for classes. The Laboratory paid for the classes, and Kathy administered exams here on site."



Dan Potter's Target Viewer maps images of a National Ignition Facility BB-sized target in a three-dimensional sphere, allowing users to zoom around the target in a Web-based application similar to Google Earth.

While working on her certificate, Chen applied her new skills to a project that examines how viruses evolve and mutate both in natural hosts and in laboratory cell lines. Her work includes searching for markers that enable viruses to transmit from one host to another. Chen believes it's important to learn new skills by taking on varied projects and working with others doing cutting-edge research. "The Education Assistance Program prepared me to enter a new area of research and gave me the opportunity to learn from professors renowned in their fields," she says. "It's a privilege to have this program available."

Master's Project on Target at NIF

Computer scientist Dan Potter came to Livermore as an undergraduate summer student, while completing his computer science degree and applying to graduate schools. "Coming here really opened my eyes, and working at NIF [the National Ignition Facility], the world's largest and most energetic laser, has been an amazing experience," he says. Potter continued working at NIF through his winter-term graduation, intending to start graduate school at UC Davis the following fall. But things changed. "NIF's contributions to energy research made me realize I wanted to continue my efforts at NIF," says Potter. "My decision to stay was met with enthusiasm, but I also was strongly encouraged to pursue an advanced degree. Luckily, I could do both."

Potter applied for a full-time position at NIF and deferred enrollment at UC Davis. He says, "When the time came to begin the UC Davis program and blend it with my job, Kathy made it easy. I filled out the paperwork, met with my managers to justify my education plan, and enrolled." Soon after he started his course work, Education Assistance moved from the TV system to Web-based learning. Potter found the new system convenient: He could view lectures on his computer on his own time, versus scheduling classes to attend at noon onsite or taking VHS tapes home for later viewing.

For his master's project, Potter created a Web-based application for visualizing NIF target data. He says, "Just as Google Earth allows one to rotate and zoom in and out over Earth's surface, my application, Target Viewer, allows NIF scientists to interactively explore target surfaces." Previously, NIF scientists had to examine hundreds of target surface images, either in small static groups or one at a time. Target Viewer replaced this onerous process. Potter used WebGL—a Web-based graphics library that enables real-time three-dimensional rendering capabilities to run within various Web browsers. In addition to zooming and

(left) Landruff Trent of Mechanical Engineering assists employees taking a microwave-transmitted TV course in the 1970s. (below) Today, employees can watch a Web-based streaming lecture on a computer from their home or office (shown here Haiyin Chen).

moving about a target's surface, Target Viewer users can simultaneously compare two target surfaces or examine one target from multiple perspectives. The NIF target group began using Target Viewer instantly. "It was a worthwhile experience," says Potter. "I was doing grad work and supporting the project as well as getting immediate feedback from users."

As is often true, the experience had extended benefits. Not only did Potter obtain his master's degree, he also developed a useful tool that was applied. Furthermore, he gained visibility at the Laboratory, writing a paper and presenting a poster at last year's International Atomic Energy Association's meeting. "The project resulted in long-term benefits I had not foreseen," he says.

Potter, who gives full marks to the Education Assistance Program, says, "I don't know if I would have tackled grad school while working if the UC Davis relationship didn't exist. The program allowed me to remain part of the NIF community while earning an advanced degree, benefiting me and the Lab."

Benefits Accrue to All

Although the technology for offering courses has changed over the years, with microwave-transmitted TV giving way to Web-based streaming, the opportunity to learn and earn degrees while on the job continues to play a significant role in recruiting and retention. Monika Witte, deputy division leader of Laser Systems Engineering and Operations and chair of the Laboratory's Student Policy Committee, believes that the benefit of this education to Lawrence Livermore is tremendous.

"These individuals bring forward both Lab experience and new mission-oriented technical or organizational skills," she says. "Employees who participate are fortunate to advance their careers with both the skills gained from work experience and from continued education. I believe employees should seriously consider taking advantage of this Laboratory-sponsored education program."

—Ann Parker

Key Words: Education Assistance Program, continuing education, distance learning.

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In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Staged Combustion with Piston Engine and Turbine Engine Supercharger

Larry E. Fischer, Brian L. Anderson, Kevin C. O'Brien
U.S. Patent RE42,875 E
November 1, 2011
A combustion engine method provides increased fuel efficiency and reduces polluting exhaust emissions by burning fuel in a two-stage combustion system. In the first stage, fuel is combusted in a piston engine, producing exhaust gases. In the second stage, fuel contained in these exhaust gases is combusted in a turbine engine. The turbine engine exhaust gases are used to supercharge the piston engine.

Preparation of Membranes Using Solvent-Less Vapor Deposition Followed by In-Situ Polymerization

Kevin C. O'Brien, Stephan A. Letts, Christopher M. Spadaccini, Jeffrey C. Morse, Steven R. Buckley, Larry E. Fischer, Keith B. Wilson
U.S. Patent US 8,101,023 B2
January 24, 2012
In this system for fabricating a composite membrane from a membrane substrate, solventless vapor deposition is followed by in situ polymerization. First and second monomers are mixed in a deposition chamber and then deposited via a solventless vapor onto the membrane substrate in the chamber. The membrane substrate and the monomer mixture are heated to produce in situ polymerization and provide the composite membrane.

Large Dynamic Range Radiation Detector and Methods Thereof

Roscoe E. Marrs, Norman W. Madden
U.S. Patent 8,115,178 B2
February 14, 2012
A radiation detector comprises a scintillator and a photodiode optically coupled to the scintillator. The radiation detector also includes a bias voltage source electrically coupled to the photodiode. A first detector electrically coupled to the photodiode generates a signal that indicates the output charge level, and a second detector electrically coupled to the bias voltage source generates a signal that indicates the current level flowing through the photodiode.

Rankine–Brayton Engine Powered Solar Thermal Aircraft

Charles L. Bennett
U.S. Patent 8,132,412 B2
March 13, 2012
A Rankine–Brayton hybrid cycle heat engine on a solar thermal aircraft body produces the power needed by a propeller or other mechanism to enable sustained free flight. The engine has a thermal battery, preferably containing a mixture of lithium hydride and lithium. The battery supplies the heat for the fluid mixture. A solar concentrator, such as a reflective parabolic trough, is connected to an optically transparent section of the aircraft body to receive and concentrate solar energy from within the aircraft. A collection and transport unit collects the concentrated solar energy, and this heat is transported to the thermal battery. A solar tracker with a heliostat determines optimal alignment with the Sun, and a drive motor actuates the solar concentrator into alignment.

Shape Memory Polymer Foams for Endovascular Therapies

Thomas S. Wilson, Duncan J. Maitland
U.S. Patent 8,133,256 B2
March 13, 2012
This system for occluding a physical anomaly comprises a shape-memory material body that fits within a physical anomaly. The material body has a primary shape for occluding the anomaly and a secondary shape for being positioned in it.

Method for Warning of Radiological and Chemical Substances Using Detection Paints on a Vehicle Surface

Joseph C. Farmer
U.S. Patent 8,133,735 B2
March 13, 2012
A warning system detects corrosion or chemical and radiological substances on a vehicle surface. The system comprises a surface covered with a paint or coating that includes an indicator material. The surface is then monitored for indications of corrosion or chemical and radiological substances.

Thermal Casting of Polymers in Centrifuge for Producing X-Ray Optics

Randy M. Hill, Todd A. Decker
U.S. Patent 8,142,691 B2
March 27, 2012
An optic is produced by first placing a polymer inside a cylindrical chamber that rotates and has an outside wall. The chamber is then rotated and heated. This process forces the polymer to the outside wall of the rotating chamber. The chamber is allowed to cool, and during this time, an optic substrate with a coated surface is produced and sized.

Carbon Fuel Cells with Carbon Corrosion Suppression

John F. Cooper
U.S. Patent 8,153,328 B2
April 10, 2012
An electrochemical cell apparatus operates as either a fuel cell or a battery. It includes a cathode compartment, an anode compartment connected to the cathode compartment, and a carbon fuel-cell section connected to both the anode and cathode compartments. An effusion plate is positioned adjacent to the anode or cathode compartment. The effusion plate allows passage of carbon dioxide. Exhaust channels in the electrochemical cell direct the carbon dioxide from the cell.

Fission Meter

Mark S. Rowland, Neal J. Snyderman
U.S. Patent 8,155,258 B2
April 10, 2012
A neutron detector system discriminates fissile material from nonfissile material. The system includes a digital data-acquisition unit that collects data at a high rate and then processes the large volume of data in real time directly into information that a first responder can use to discriminate materials. The system counts neutrons from an unknown source and detects excess grouped neutrons to identify fissile material.

Awards

Seven teams of Laboratory researchers and engineers were presented with the **National Nuclear Security Administration**'s (NNSA's) **Defense Programs Award of Excellence**. **The Energy Balance Assessment and Application Team** developed and implemented physics-based models into advanced simulation and computing codes and used the new tools to perform integrated assessments of a range of systems and underground tests. **The Gas Gun Relocation Project Team** moved a two-stage gas gun from Building 341 to Building 191. **The Phoenix Mini-Generator Explosive Pulsed Power Development Team** demonstrated a significant advancement in generator flow–pulse shaping technology. **The Advanced Certification Hydro Team** successfully designed, fabricated, and executed a weapons safety hydro experiment at the Dual-Axis Radiographic Hydrodynamics Test Facility at Los Alamos National Laboratory. **The W84 SS21 Project Team**, which included members from Sandia National Laboratories and the Pantex Plant, successfully disassembled four W84 warheads. **The Collaborative Authorization Safety-Basis Total Lifecycle Environment (CASTLE) Project Team** developed, deployed, and managed CASTLE-PX, an integrated, classified, safety-basis data management tool for the engineering and analyst user community from the Pantex Plant and the design agencies: Lawrence Livermore, Los Alamos, and Sandia national laboratories. **The Barolo Subcritical Experimental Series Team**, which included members from Los Alamos, Sandia, and the Nevada Site Office, successfully executed the Barolo Subcritical Experimental Series at the Nevada National Security Site.

Laboratory physicist **Roger White** of the Weapons and Complex Integration Principal Directorate received an award from the **Defense Threat Reduction Agency** (DTRA) for his work in postdetonation nuclear forensics. White was named the **top contributor of the quarter** for the second quarter of fiscal year 2012 for integrating a multilaboratory effort to develop a prompt diagnostics research event. Funded by DTRA, the effort is developing new methods for improved forensic analysis of speed-of-light signals from a nuclear explosion. These signals are transient phenomena that can be used by forensics designers to help reconstruct, for example, information about a terrorist-detonated nuclear device.

The Laboratory has been recognized by **NNSA** for three of its environmental stewardship efforts. The **Pollution Prevention Awards** recognize performance in integrating environmental stewardship practices that help to reduce risk, protect natural resources, and enhance site operations. The Laboratory received recognition for **innovative green cleaning** at the National Ignition Facility, **Fresh@the Labs**—a farmer's market collaboration (joint award with Sandia National Laboratories/California), and the **hydrogen shuttle bus** collaborative project (joint award with Sandia/California).

Four scientists in Livermore's Physical and Life Sciences Directorate received $10 million in funding through the **Department of Energy**'s **Early Career Research Program**. The program is designed to bolster the nation's scientific workforce by providing support to exceptional researchers during the crucial early career years, when many scientists do their most formative work.

Celine Bonfils, a climate scientist in the Program for Climate Model Diagnosis and Intercomparison, earned the award for detection and attribution of regional climate change with a focus on drought precursors. **Gianpaolo Carosi**, a particle physicist, won the award for his work in search of dark matter axions using new high-frequency tunable microwave cavities. Physicist **Andreas Kemp** earned the award for large-scale modeling of intense short-pulse laser interaction for high-energy-density laser physics. Engineer **Jaime Marian** won the award for his work in computational modeling and design of radiation-tolerant materials for fusion.

The Laboratory in the News *(continued from p. 2)*

For single-molecule bioimaging, the team found that in certain cases the method might be substantially more difficult to implement than anticipated because energy transfer is surprisingly fast. In x-ray optics, they found that the damage threshold is lower than anticipated.

The team's research appeared in the May 25, 2012, edition of *Physical Review Letters*. Other participating institutions included SLAC National Accelerator Laboratory and, in Germany, the University of Duisburg-Essen, Max Planck Advanced Study Group at the Centre for Free-Electron Laser Science, Max Planck Institute for Medical Research, and Max Planck Institute for Nuclear Physics.

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Improving the Efficiency of the Biofuel Production Cycle

Using new experimental methods and computational analysis, a team of scientists from the Joint BioEnergy Institute, led by Lawrence Livermore's Michael Thelen, discovered how certain bacteria can tolerate man-made toxic chemicals used in making biofuels. While sugars stored within the plant cell wall, known as lignocellulose, are plentiful enough to supply most energy needs on the planet, their extraction is difficult and requires chemical pretreatment followed by enzymatic digestion using microorganisms. Ionic liquids—salty solvents—improve the digestibility of lignocellulose, but they are toxic to bacteria used in subsequent conversion steps.

Microbes found in natural environments, such as decomposing forest soils, produce highly efficient enzymes to degrade lignocellulose and often can adapt to stressful changes in the environment. By harnessing the positive traits of these native bacteria, researchers can engineer existing laboratory strains for more effective biofuel processing in the presence of toxic solvents. Thelen and his colleagues isolated *Enterobacter lignolyticus* strain SCF1, a bacterium that can degrade lignocellulose from plant biomass, and found that SCF1 grows well in relatively high concentrations of an ionic liquid used for lignocellulose pretreatment even though this chemical is highly toxic to other bacterial species.

"We studied how SCF1 tolerates this ionic liquid by using high-throughput growth assays, performing composition analysis of the bacterial cell membrane, and determining the genes that are differentially expressed when SCF1 cells are exposed to an ionic liquid," says Thelen. The team mapped these analyses onto the known metabolic reactions identified in the SCF1 genome sequence. Those results indicated that the bacteria would resist the toxic effects of an ionic liquid if the composition of membranes is adjusted to reduce cell permeability and a transport protein is increased enough to pump the toxic chemical out of the cell before damage occurs.

"These results will be used as a foundation for genetic engineering of ionic liquid–tolerant microorganisms for a more efficient biofuel production process," says Thelen. The team's research appeared in the May 14, 2012, online edition of the *Proceedings of the National Academy of Sciences*. Other institutions involved in this research effort include Lawrence Berkeley National Laboratory, Joint Genome Institute, and Sandia National Laboratories.

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Mysteries of Cell Repair Selected Editor's Choice

Laboratory researcher Salustra Urbin and colleagues have determined that a previously presumed relationship between RAD51 (a family of proteins) and DNA repair may not exist after all. The research team demonstrated, for the first time, that cell survival and RAD51D repair can be separate activities. The journal *Environmental and Molecular Mutagenesis* selected the team's research paper as the editor's choice and cover story for the March 2012 issue.

Research shows that double-stranded DNA breaks are very dangerous. In humans, breaks can occur for many reasons, ranging from exposure to dangerous chemicals, ionizing radiation, cigarette smoke, or ultraviolet radiation from the Sun. Breaks in DNA either lead to the death of the cell or DNA mutations that can cause cancer. Until now, scientists believed that certain proteins, known as RAD51, were required to come together to repair these breaks in the DNA.

"DNA repair is a part of daily life," Urbin says. "Barring any accidents or other diseases, all of us die from cancer. What we've discovered is that we probably know less about how cells repair themselves than we thought we did." The team's research is funded by grants from the National Institutes of Health's National Cancer Institute, the Department of Health and Human Services, and the Swedish Cancer Society.

Contact: Salustra Urbin (925) 422-9320 (urbin2@llnl.gov).

Abstract

A Home for Energetic Materials and Their Experts

The Energetic Materials Center (EMC) is the Laboratory's focal point for research and development of explosives, propellants, and pyrotechnics. In 2008, the National Nuclear Security Administration (NNSA) named Lawrence Livermore its R&D Center of Excellence for high explosives because of EMC and the people and research facilities that support it. EMC provides expertise on energetic materials to the Department of Energy, NNSA, Department of Defense, Department of Homeland Security, Transportation Security Administration, Federal Bureau of Investigation, and other law-enforcement and government organizations. The center is located at the High Explosives Applications Facility, where the majority of high-explosives synthesis, formulation, experiment, and theory are performed at Livermore. Energetic materials are fabricated in bulk quantities at Site 300, located 24 kilometers away from the Laboratory's main site.

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Coming Next Issue

Building a 21st-Century Vaccine

Laboratory scientists have developed a "platform" that uses nanolipoprotein particles to hold and deliver vaccines against infectious diseases.

Also in September

• High-energy-density physics campaigns have demonstrated the National Ignition Facility's ability to perform precise experiments relevant to stockpile stewardship and basic science.

• In simulations to commission the Sequoia supercomputer, Livermore and IBM scientists have developed a highly scalable electrophysiological model of the human heart.

• Laboratory engineers and computational scientists are extending the capability of proven simulation codes for addressing key national security problems.

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